Superheated Crystals: Thermodynamic Properties, Stability Criteria, Homogeneous Nucleation and Melting

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The theoretical and experimental data are reviewed and original results are presented concerning theoretical and simulation aspects of the thermophysical properties of superheated solids: equation of state, thermodynamic, mechanic and kinetic limits of stability lifetime distribution, activation energy and rate of the homogeneous nucleation, dynamics of melting and state of the fluid formed. Both quasi-stationary metastable solid state and peculiarities of solid superheating and decay under time-varying external conditions are treated. The molecular dynamics method is used for the study of model crystals. The simulation peculiarities are treated, which are related to the Lyapunov instability which is inherent to the many-particle dynamic molecular systems; the concept of dynamical memory time is exploited. The Lennard-Jones and uniform soft-sphere pair potentials were chosen for the interparticle interaction. The correspondence of various stability criteria to each other, the character and time of the process of the melting transition from superheated crystal to fluid state are discussed. Fast (nanoseconds) electric explosion of thin wires at high rate of energy input is considered. The initial stage of the process is treated as superheating of a solid metal. The theoretical predictions and experimental findings are compared for (a) the dependence of the maximum energy deposited and the column uniformity on the heating rate, (b) the scatter of deposited energies for the same heating rate, (c) the jump of the expansion speed at the moment of melting, and (d) the field influence.